Connecting via Winsock to STN

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Welcome to STN International! Enter x:x
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LOGINID:ssspta1201txs

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
     1
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
        SEP 01
                New pricing for the Save Answers for SciFinder Wizard within
                 STN Express with Discover!
        OCT 28 KOREAPAT now available on STN
NEWS
      5 NOV 30 PHAR reloaded with additional data
NEWS
      6 DEC 01 LISA now available on STN
NEWS
      7 DEC 09 12 databases to be removed from STN on December 31, 2004
NEWS
      8 DEC 15
NEWS
                MEDLINE update schedule for December 2004
     9 DEC 17
NEWS
                ELCOM reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
      10 DEC 17
                 COMPUAB reloaded; updating to resume; current-awareness
NEWS
                 alerts (SDIs) affected
NEWS
      11 DEC 17
                 SOLIDSTATE reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
NEWS
      12 DEC 17
                 CERAB reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
      13 DEC 17
                THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS
      14 DEC 30
NEWS
                EPFULL: New patent full text database to be available on STN
      15 DEC 30
NEWS
                CAPLUS - PATENT COVERAGE EXPANDED
NEWS 16 JAN 03
                No connect-hour charges in EPFULL during January and
                 February 2005
NEWS
      17 JAN 26
                 CA/CAPLUS - Expanded patent coverage to include the Russian
                 Agency for Patents and Trademarks (ROSPATENT)
      18 FEB 10
                 STN Patent Forums to be held in March 2005
NEWS
                 STN User Update to be held in conjunction with the 229th ACS
NEWS
      19 FEB 16
                 National Meeting on March 13, 2005
NEWS EXPRESS
              JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
```

MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

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NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)
```

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FILE 'HOME' ENTERED AT 16:56:47 ON 16 FEB 2005

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.42 0.42

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 16:57:40 ON 16 FEB 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5 DICTIONARY FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5

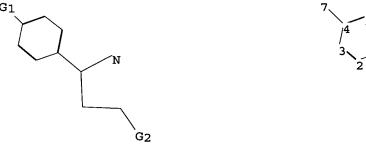
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\106291081.str



chain nodes : 7 8 9 10 11 ring nodes : 3 4 5 6 chain bonds : 1-8 4-7 8-9 8-10 10-11 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 4-7 8-9 11-12 exact bonds :

R

1-8 8-10 10-11 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

G1:0,S

G2:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS

30 ANSWERS

T.1 STRUCTURE UPLOADED

=> s 11

SAMPLE SEARCH INITIATED 16:57:57 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 6765 TO ITERATE

14.8% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\* PROJECTED ITERATIONS: 130370 TO 140230 PROJECTED ANSWERS: 3205 TO 4913

30 SEA SSS SAM L1 L2

=> s l1 ful

FULL SEARCH INITIATED 16:59:48 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 135281 TO ITERATE

100.0% PROCESSED 135281 ITERATIONS 4080 ANSWERS

SEARCH TIME: 00.00.02

4080 SEA SSS FUL L1 T.3

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 167.78 FULL ESTIMATED COST 168.20

FILE 'CAPLUS' ENTERED AT 17:07:11 ON 16 FEB 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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SINCE FILE

ENTRY

1.35

TOTAL SESSION

169.55

FILE COVERS 1907 - 16 Feb 2005 VOL 142 ISS 8 FILE LAST UPDATED: 15 Feb 2005 (20050215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 680 L3

=> file reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 17:08:57 ON 16 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5 DICTIONARY FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\106291082.str

chain nodes : 7 8 9 10 11 12 ring nodes :

1 2 3 4 5 6

chain bonds :

1-8 4-7 8-9 8-10 10-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds : 4-7 8-9 11-12 exact bonds : 1-8 8-10 10-11 normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:0,S

G2:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:CLASS

L5 STRUCTURE UPLOADED

=> s 15

SAMPLE SEARCH INITIATED 17:09:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6724 TO ITERATE

14.9% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 129565 TO 139395

PROJECTED ANSWERS: 2347 TO 3839

L6 23 SEA SSS SAM L5

=> s 15 ful

FULL SEARCH INITIATED 17:09:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 134869 TO ITERATE

100.0% PROCESSED 134869 ITERATIONS 3664 ANSWERS

SEARCH TIME: 00.00.02

L7 3664 SEA SSS FUL L5

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

23 ANSWERS

FULL ESTIMATED COST 161.33 330.88

FILE 'CAPLUS' ENTERED AT 17:09:31 ON 16 FEB 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 16 Feb 2005 VOL 142 ISS 8 FILE LAST UPDATED: 15 Feb 2005 (20050215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17 L8 649 L7

=> d 18 ibib hitstr 1-10

L8 ANSWER 1 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:36482 CAPLUS

DOCUMENT NUMBER:

142:133207

TITLE:

SOURCE:

Enzymic stereospecific and enantiomeric enrichment of

β-amino acids

INVENTOR(S):

Chase, Matthew; Clayton, Robert; Landis, Bryan;

Banerjee, Amit

PATENT ASSIGNEE(S):

Pharmacia Corporation, USA

U.S. Pat. Appl. Publ., 44 pp.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA.	PATENT NO.					KIND DATE			i	APPL	ICAT:		DATE					
US	2005009151				A1 200501:			0113	1	US 2	004-	20040622						
WO	2005	0056	33		A2		20050120		1	WO 2	004-3	IB21	83	20040630				
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DΖ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NA,	NI,	
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ΥU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	
							RU,											
							GR,											
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	
		SN,	TD,	TG														
PRIORITY	Y APP	LN.	INFO	. :					1	US 2	003-	4860	32P		P 20	0030	710	
									1	US 2	003-	4996	22P	:	P 20	0030	902	

## IT 5678-45-5P

RL: BCP (Biochemical process); BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); PROC (Process);

RACT (Reactant or reagent)

(enzymic stereospecific and enantiomeric enrichment of  $\beta$ -amino acids)

RN 5678-45-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -amino-4-methoxy- (9CI) (CA INDEX NAME)

IT 213192-51-9

RL: BCP (Biochemical process); RCT (Reactant); BIOL (Biological study);
PROC (Process); RACT (Reactant or reagent)

(enzymic stereospecific and enantiomeric enrichment of  $\beta$ -amino acids)

RN 213192-51-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -amino-4-phenoxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH}_2 \\ | \\ \text{CH-CH}_2\text{-CO}_2\text{H} \end{array}$$

L8 ANSWER 2 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:1044920 CAPLUS

DOCUMENT NUMBER: 142:134184

TITLE: A highly stereoselective addition of the anion derived

from α-diazoacetamide to aromatic N-tosylimines

AUTHOR(S): Zhao, Yonghua; Ma, Zhihua; Zhang, Xiaomei; Zou,

Yaping; Jin, Xianglin; Wang, Jianbo

CORPORATE SOURCE: Key Laboratory of Bioorganic Chemistry and Molecular

Engineering of the Ministry of Education, Peking University, Beijing, 100871, Peop. Rep. China

SOURCE: Angewandte Chemie, International Edition (2004),

43(44), 5977-5980

CODEN: ACIEF5; ISSN: 1433-7851 Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

IT 825627-59-6P

PUBLISHER:

RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective preparation of chiral Me aminohydroxyesters via base-promoted condensation of chiral diazocarbonyl compds. with

tosylimines followed by removal of chiral auxiliary, diazo oxidation and

stereoselective ketone reduction)

RN 825627-59-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry. Rotation (-).

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

ANSWER 3 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:1033523 CAPLUS

DOCUMENT NUMBER:

142:2109

TITLE:

Preparation of copper salts of organic acids as

agrochemical and technical fungicides

INVENTOR(S):

Gusmeroli, Marilena; Mormile, Silvia Maria; Gironda,

APPLICATION NO.

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DATE

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Ramona; Mirenna, Luigi; Osti, Samuele

PATENT ASSIGNEE(S):

SOURCE:

Isagro S.p.A., Italy PCT Int. Appl., 71 pp.

DATE

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CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

KIND

\_\_\_\_

FAMILY ACC. NUM. COUNT:

\_\_\_\_\_

PATENT INFORMATION:

PATENT NO.

	WO	2004	1030	74		A1 20041202				1	WO 20	004-1	EP54	90	20040508					
		W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	ВG,	BR,	BW,	BY,	ΒZ,	CA,	CH,		
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,		
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NA,	NI,		
			NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,		
			ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	ŪĠ,	US,	UΖ,	VC,	VN,	ΥU,	ZA,	ZM,	ZW		
		RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	ŪG,	ZM,	ZW,	AM,		
			ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
			EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	ΙE,	IT,	LU,	MC,	ΝL,	PL,	PT,	RO,	SE,		
			SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,		
			SN,	TD,	TG															
PRIO	RITY	APP	LN.	INFO	. :						IT 20	003-1	MI10	20	i	A 2	0030	521		
IT	798	557-	58-1	DP,	copp	er c	ompl	exes	798	557-	59-21	DP, (	copp	er						
		plex																		
	RL:	AGR	(Ag	ricu	ltur	al u	se);	IMF	(In	dust:	rial	man	ufac	ture	); B	$10\Gamma$	(Bio	logical		
	stu	dy);	PRE	P (P	repa	ratio	on);	USE	S (U	ses)										
		(pre	para	tion	as	agro	chem	. and	d te	ch.	fung	icid	e)							
RN		557-																		
CN	CN Propanedioic acid, [amino(4-hydroxy-3-methoxyphenyl)methyl] - (9CI) (CA																			
	IND	EX N	AME)																	

$$\begin{array}{c|c} & \text{H}_2\text{N} & \text{CO}_2\text{H} \\ & & | & | \\ \text{CH} - \text{CH} - \text{CO}_2\text{H} \\ \\ \text{HO} & \\ & \text{OMe} \end{array}$$

RN 798557-59-2 CAPLUS

CN Propanedioic acid, [amino(3,4-dimethoxyphenyl)methyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{H}_2\text{N} & \text{CO}_2\text{H} \\ & & \\ & \text{CH--CH--CO}_2\text{H} \\ \\ & \text{OMe} \end{array}$$

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:995769 CAPLUS

DOCUMENT NUMBER:

141:424300

TITLE:

P-chiral phospholanes and phosphocyclic compounds and

their use in asymmetric catalytic reactions

INVENTOR(S):

Zhang, Xumu; Tang, Wenjun

PATENT ASSIGNEE(S):

The Penn State Research Foundation, USA

SOURCE:

U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U.S.

Ser. No. 291,232.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004229846	A1	20041118	US 2004-856014	20040528
US 2003144137	A1	20030731	US 2002-291232	20021108
PRIORITY APPLN. INFO.:			US 2001-336939P P	20011109
			US 2002-291232 A	2 20021108

OTHER SOURCE(S): CASREACT 141:424300

IT 434957-82-1P 479550-67-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of P-chiral phospholanes and phosphocyclic compds. and their use in transition metal catalyzed asym. reactions)

RN 434957-82-1 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -(acetylamino)-4-methoxy-, methyl ester,  $(\beta S)$ -(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 479550-67-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -(acetylamino)-4-(phenylmethoxy)-, methyl ester, ( $\beta$ S)- ( $\beta$ CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L8 ANSWER 5 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:989192 CAPLUS

DOCUMENT NUMBER: 142:113654

TITLE: Product-catalyzed Mannich-type reaction between

trimethylsilyl enolates and N-tosylaldimines

AUTHOR(S): Takahashi, Eiki; Fujisawa, Hidehiko; Mukaiyama,

Teruaki

CORPORATE SOURCE: Center for Basic Research, The Kitasato Institute

(TCI), Tokyo, 114-0003, Japan

SOURCE: Chemistry Letters (2004), 33(11), 1426-1427

CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal LANGUAGE: English

IT 641614-50-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(alkoxide-initiated autocatalytic Mannich-type reaction between

trimethylsilyl enolates and N-tosylaldimines)

RN 641614-50-8 CAPLUS

CN Benzenepropanoic acid, 4-methoxy- $\alpha$ ,  $\alpha$ -dimethyl- $\beta$ -[[(4-

methylphenyl)sulfonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:965208 CAPLUS

DOCUMENT NUMBER: 141:411087

TITLE: Preparation of chiral Bronsted catalysts in asym.

synthesis and asym. Mannich, aza-Diels-Alder reaction,

hydrophosphorylation therewith

INVENTOR(S): Akiyama, Takahiko

PATENT ASSIGNEE(S): Toagosei Co., Ltd., Japan SOURCE: PCT Int. Appl., 103 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIN	<b>D</b> 1	DATE		APPLICATION NO.						DATE			
WO 2004096753					7.1	-	2004	1111	1	WO 2	004-	TP56	20040420					
WO																CA,		
	w:																	
		LK,	LR,	LS,	LT,	LU,	LV,	MΑ,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
		NO,	ΝZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	ŪĠ,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	
																SE,		
		SK,	TR,	BF,	вJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	
		TD,																
	R₩:	GE, LK, NO, TJ, BW, BY, ES, SK,	GH, LR, NZ, TM, GH, KG, FI, TR,	GM, LS, OM, TN, GM, KZ, FR,	HR, LT, PG, TR, KE, MD, GB,	HU, LU, PH, TT, LS, RU, GR,	ID, LV, PL, TZ, MW, TJ, HU,	IL, MA, PT, UA, MZ, TM, IE,	IN, MD, RO, UG, SD, AT, IT,	IS, MG, RU, US, SL, BE, LU,	JP, MK, SC, UZ, SZ, BG, MC,	KE, MN, SD, VC, TZ, CH, NL,	KG, MW, SE, VN, UG, CY, PL,	KP, MX, SG, YU, ZM, CZ, PT,	KR, MZ, SK, ZA, ZW, DE, RO, MR,	ZM, AM, DK, SE,	LC NI SY AZ EE SI SN	

PRIORITY APPLN. INFO.: JP 2003-121706 A 20030425

OTHER SOURCE(S): MARPAT 141:411087 IT 694472-15-6P 694472-22-5P 791121-11-4P

791121-31-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of chiral Bronsted catalysts in asym. synthesis and asym. Mannich, aza-Diels-Alder reaction, hydrophosphorylation therewith)

RN 694472-15-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -[(2-hydroxyphenyl)amino]-4-methoxy- $\alpha$ -

methyl-, ethyl ester, (αR, βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 694472-22-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -[(2-hydroxyphenyl)amino]-4-methoxy- $\alpha$ -(phenylmethyl)-, ethyl ester, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 791121-11-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -[(2-hydroxyphenyl)amino]-4-methoxy- $\alpha$ ,  $\alpha$ -dimethyl-, methyl ester, ( $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 791121-31-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -[(2-hydroxyphenyl)amino]-4-methoxy- $\alpha$ -[(triphenylsilyl)oxy]-, methyl ester, ( $\alpha$ R, $\beta$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:870347 CAPLUS

DOCUMENT NUMBER: 142:55710

TITLE: Synthesis of Monodentate Chiral Spiro Phosphonites and

the Electronic Effect of Ligand in Asymmetric

Hydrogenation

AUTHOR(S): Fu, Yu; Hou, Guo-Hua; Xie, Jian-Hua; Xing, Liang;

Wang, Li-Xin; Zhou, Qi-Lin

CORPORATE SOURCE: State Key Laboratory and Institute of Elemento-Organic

Chemistry, Nankai University, Tianjin, 300071, Peop.

Rep. China

SOURCE: Journal of Organic Chemistry (2004), 69(23), 8157-8160

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

IT 810670-02-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of monodentate chiral spiro phosphonites and electronic

effect of ligand in asym. hydrogenation)

RN 810670-02-1 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -(acetylamino)-4-methoxy-, methyl ester,

(βR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

NHAC O OMe

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:863000 CAPLUS

DOCUMENT NUMBER: 142:23000

TITLE: A simple route to  $\beta$ -aminomethylketones AUTHOR(S): Zawadzki, Stefan; Zwierzak, Andrzej

CORPORATE SOURCE: Institute of Organic Chemistry, Technical University

(Politechnika), Lodz, 90-924, Pol.

Tetrahedron Letters (2004), 45(46), 8505-8506 SOURCE:

CODEN: TELEAY; ISSN: 0040-4039

Elsevier B.V. PUBLISHER:

DOCUMENT TYPE: Journal English LANGUAGE:

TT 801290-81-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of β-aminomethylketones by base-catalyzed Michael-type addition of sodium t-Bu acetoacetate to N-Boc imines)

801290-81-3 CAPLUS RN

Benzenepropanoic acid,  $\alpha$ -acetyl- $\beta$ -[[(1,1-CN dimethylethoxy)carbonyl]amino]-4-methoxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS 21 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:848408 CAPLUS

DOCUMENT NUMBER:

142:23050

TITLE:

Solvent-free imino-aldol three-component couplings on

a conveniently-prepared and reusable phosphoric

acid-silica gel support

AUTHOR (S):

Lock, Sandra; Miyoshi, Norikazu; Wada, Makoto

CORPORATE SOURCE:

Department of Chemistry, Faculty of Integrated Arts

and Sciences, University of Tokushima, Tokushima,

770-8502, Japan

SOURCE:

Chemistry Letters (2004), 33(10), 1308-1309

CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER:

Chemical Society of Japan

DOCUMENT TYPE:

Journal

English

LANGUAGE: IT 745033-30-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of  $\beta$ -amino esters, and ketones via three-component Mannich coupling reaction of aldehydes with anilines and silyl enol ethers

mediated by silica supported phosphoric acid)

RN745033-30-1 CAPLUS

Benzenepropanoic acid, 4-methoxy- $\alpha$ ,  $\alpha$ -dimethyl- $\beta$ -CN(phenylamino) -, methyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 10 OF 649 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:824045 CAPLUS

DOCUMENT NUMBER: 141:332476

TITLE: Process for preparation of chiral  $\beta$ -amino acid

derivatives

INVENTOR(S): Dreher, Spencer D.; Ikemoto, Norihiro; Njolito,

Eugenia; Rivera, Nelo R.; Tellers, David M.; Xiao, Yi

PATENT ASSIGNEE(S): Merck & Co., Inc, USA SOURCE: PCT Int. Appl., 39 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND		DATE		APPLICATION NO.							DATE			
						-													
WO	WO 2004085661				A2		2004	1007	1	WO 2	004-1		20040319						
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,		
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JΡ,	ΚE,	KG,	KΡ,	KR,	ΚZ,	LC,		
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NA,	NI,		
		NO,	NZ,	OM,	PG,	PH,	ΡL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	sĸ,	SL,	SY,		
		ТJ,	TM,	TN,	TR,	TT,	TZ,	ŲΑ,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,		
		BY,	KG,	KZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,		
		ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	SI,		
		SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ΜL,	MR,	ΝE,	SN,		
		TD,	TG																

PRIORITY APPLN. INFO.:

US 2003-457128P P 20030324 US 2003-511210P P 20031015

OTHER SOURCE(S): CASREACT 141:332476; MARPAT 141:332476

IT 769195-23-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (asym. synthesis of chiral  $\beta\text{-amino}$  acid derivs. via addition of phenylglycine amide to triazolopyrazinyl  $\beta\text{-ketoesters}$ , followed by catalytic hydrogenation of enamines and catalytic hydrogenolysis)

RN 769195-23-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -[[(1S)-2-amino-2-oxo-1-phenylethyl]amino]-4-methoxy-, methyl ester, ( $\beta$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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SINCE FILE TOTAL ENTRY SESSION 46.95 377.83

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February 2005

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NEWS 18 FEB 10 STN Patent Forums to be held in March 2005

NEWS 19 FEB 16 STN User Update to be held in conjunction with the 229th ACS National Meeting on March 13, 2005

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

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Page 17

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chain nodes : 7 8 9 10 11 12 22 23 24 25 26 27 28 29 ring nodes : 1 2 3 4 5 6 16 17 18 19 20 21 chain bonds : 1-8 4-7 7-25 8-9 8-10 9-23 9-24 10-11 11-12 12-18 21-22 25-26 25-27 27-28 27-29 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 exact/norm bonds : 4-7 7-25 8-9 9-24 11-12 12-18 25-26 25-27 27-28 27-29 exact bonds : 1-8 8-10 9-23 10-11 21-22 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 isolated ring systems : containing 1 :

G1:0,S

G2:0,S,N

## Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS

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PROJECTED ITERATIONS: 11 TO 389

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PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> s 11 ful

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FULL SCREEN SEARCH COMPLETED - 181 TO ITERATE

100.0% PROCESSED 181 ITERATIONS 27 ANSWERS

SEARCH TIME: 00.00.01

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L4 6 L3

=> d l4 ibib hitstr abs 1-6

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:291183 CAPLUS

DOCUMENT NUMBER: 140:315087

TITLE: Pharmaceuticals containing (hydroxybenzyl)amines as

acetylcholine esterase inhibitors and selective

serotonin reuptake inhibitors

INVENTOR(S): Koyama, Kazuo; Marumoto, Masashi; Toda, Seihiro;

Suzuki, Keiko; Furumoto, Hiroshi

PATENT ASSIGNEE(S): BTG International Ltd., UK

SOURCE: Jpn. Kokai Tokkyo Koho, 141 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 2004107322 A2 20040408 JP 2003-200434 20030723
PRIORITY APPLN. INFO.: JP 2002-214641 A 20020724

OTHER SOURCE(S):

MARPAT 140:315087

IT 444646-40-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of benzylamines as acetylcholine esterase inhibitors and selective serotonin reuptake inhibitors for treatment of diseases)

RN 444646-40-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

#### IT 474295-88-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzylamines as acetylcholine esterase inhibitors and selective serotonin reuptake inhibitors for treatment of diseases)

RN 474295-88-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

AB Title pharmaceuticals, useful for treatment of Alzheimer's disease, depression, etc., contain R1C(:X1)X2C6H4CH(NR2R3)AEArom [I: R1 = C1-6 alkyl, (di)(C1-6 alkyl)amino, N-containing saturated heterocyclyl; R2, R3 = H, C1-6 alkyl; Arom = aryl, (un)substituted (hetero)aryl; A = C1-6 alkylene; E = bond, O, S, NR4; R4 = H, C1-7 alkanoyl; X1, X2 = O, S], pharmacol.

acceptable salts, or esters. Thus, I  $\{R1(C:X1) = N,N-dimethylcarbamoyl, R2 = Me, R3 = H, A = (CH2)2, E = O, Arom = 4-ClPh] inhibited serotonin reuptake and acetylcholine esterase with IC50 values of 210 and 493 nM, resp.$ 

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2003:781444 CAPLUS

DOCUMENT NUMBER:

140:192823

TITLE:

Pharmacological characterization of RS-1259, an orally active dual inhibitor of acetylcholinesterase and serotonin transporter, in rodents: Possible treatment

of Alzheimer's disease

AUTHOR (S):

Abe, Yasuyuki; Aoyagi, Atsushi; Hara, Takao; Abe, Kazumi; Yamazaki, Reina; Kumagae, Yoshihiro; Naruto, Shunji; Koyama, Kazuo; Marumoto, Shinji; Tago, Keiko; Toda, Narihiro; Takami, Kazuko; Yamada, Naho; Ori,

Mayuko; Kogen, Hiroshi; Kaneko, Tsugio

CORPORATE SOURCE:

Neuroscience and Immunology Research Laboratories,

Sankyo Co., Ltd., Tokyo, 140-8710, Japan

SOURCE:

Journal of Pharmacological Sciences (Tokyo, Japan)

(2003), 93(1), 95-105

CODEN: JPSTGJ; ISSN: 1347-8613 Japanese Pharmacological Society

PUBLISHER:
DOCUMENT TYPE:

Journal

LANGUAGE:

English

IT 444667-97-4, RS 1259

RL: ADV (Adverse effect, including toxicity); DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pharmacol. characterization of RS-1259, dual inhibitor of acetylcholinesterase and serotonin transporter, in comparison with other inhibitors in rats and possible treatment of Alzheimer's disease)

RN 444667-97-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, (2E)-2-butenedioate (2:1) (9CI) (CAINDEX NAME)

CM 1

CRN 444667-96-3 CMF C19 H23 N3 O5

Absolute stereochemistry.

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

A dual inhibitor of acetylcholinesterase (AChE) and serotonin transporter AΒ (SERT), RS-1259, was newly synthesized. RS-1259 simultaneously inhibited ACHE and SERT in the brain following an oral administration in mice and rats. Actual simultaneous elevation of extra-cellular levels of 5-HT and ACh in the rat hippocampus was confirmed by microdialysis. The compound was as effective as SERT inhibitors such as fluoxetine and fluvoxamine in a 5-hydroxytryptophan-enhancing test in mice. Spatial memory deficits in the two-platform task of a water maze in aged rats were ameliorated by RS-1259 as well as donepezil. Both RS-1259 and donepezil increased the awake episodes in the daytime EEG of rats. Although RS-1259 was weaker than donepezil in enhancing central cholinergic transmission, as observed by ACh elevation in the hippocampus and memory enhancement in aged rats, the efficacy of RS-1259 on the consciousness level, which reflects the whole activity in the brain, was almost the same as that of donepezil. results suggest that both cholinergic and serotonergic systems are involved in maintaining brain arousal and that a dual inhibitor of AChE and SERT may be useful for the treatment of cognitive disorders associated with reduced brain activity such as in Alzheimer's disease.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:728107 CAPLUS

DOCUMENT NUMBER: 140:128263

TITLE: A conformational restriction approach to the

development of dual inhibitors of acetylcholinesterase

and serotonin transporter as potential agents for

Alzheimer's disease

AUTHOR(S): Toda, Narihiro; Tago, Keiko; Marumoto, Shinji; Takami,

Kazuko; Ori, Mayuko; Yamada, Naho; Koyama, Kazuo; Naruto, Shunji; Abe, Kazumi; Yamazaki, Reina; Hara, Takao; Aoyagi, Atsushi; Abe, Yasuyuki; Kaneko, Tsugio;

Kogen, Hiroshi

CORPORATE SOURCE: Exploratory Chemistry Research Laboratories, Sankyo

Co., Ltd., Shinagawa-ku, Tokyo, 140-8710, Japan Bioorganic & Medicinal Chemistry (2003), 11(20),

4389-4415

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

IT 474295-96-0P 474295-97-1P 474295-98-2P

474296-05-4P

SOURCE:

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of dimethylcarbamic acid 2-methyl-1-[2-(4-nitrophenoxy)ethyl]-2,3-dihydro-1H-benzo[c]azepin-7-yl ester and related compds. as dual

inhibitors of acetylcholinesterase and serotonin transporter)

RN 474295-96-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]-3-(methoxymethoxy)phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474295-97-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]-3-hydroxyphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474295-98-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]-3-ethenylphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$H_2C$$
 $HN$ 
 $OBu-t$ 
 $NO_2$ 
 $Me_2N$ 

RN 474296-05-4 CAPLUS

CN Methanesulfonic acid, trifluoro-, 5-[[(dimethylamino)carbonyl]oxy]-2-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

GI

Alzheimer's disease (AD) has been treated with acetylcholinesterase (AChE) inhibitors such as donepezil. However, the clin. usefulness of AChE inhibitors is limited mainly due to their adverse peripheral effects. Depression seen in AD patients has been treated with serotonin transporter (SERT) inhibitors. The authors considered that combining SERT and AChE inhibition could improve the clin. usefulness of AChE inhibitors. In a previous paper, the authors found a potential dual inhibitor of AChE (IC50 = 101 nM) and SERT (IC50 = 42 nM), but its AChE inhibition activity was less than donepezil (IC50 = 10 nM). Here, the authors report the conformationally restricted (R)-I considerably enhanced inhibitory activity against AChE (IC50 = 14 nM) and SERT (IC50 = 6 nM).

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 26 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

2003:251390 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 139:173164

Design, synthesis and structure-Activity relationships TITLE:

of dual inhibitors of acetylcholinesterase and serotonin transporter as potential agents for

Alzheimer's disease

AUTHOR (S):

Toda, Narihiro; Tago, Keiko; Marumoto, Shinji; Takami, Kazuko; Ori, Mayuko; Yamada, Naho; Koyama, Kazuo; Naruto, Shunji; Abe, Kazumi; Yamazaki, Reina; Hara,

Takao; Aoyagi, Atsushi; Abe, Yasuyuki; Kaneko, Tsugio;

Kogen, Hiroshi

CORPORATE SOURCE: Exploratory Chemistry Research Laboratories, Sankyo

Co., Ltd., Shinagawa-ku, Tokyo, 140-8710, Japan Bioorganic & Medicinal Chemistry (2003), 11(9),

SOURCE: Bioorgani 1935-1955

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:173164
IT 444644-44-4P 444645-31-2P 444667-96-3P

474295-89-1P 578730-21-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis and structure-Activity relationships of dual inhibitors of acetylcholinesterase and serotonin transporter as potential agents for Alzheimer's disease)

RN 444644-44-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ || \\ || \\ NHMe \\ | \\ CH-CH_2-CH_2-O \end{array}$$

● HCl

RN 444645-31-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(ethylamino)-3-(4nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444667-96-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474295-89-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 578730-21-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NHMe} \\ \text{NHMe} \\ \text{CH-CH}_2\text{-CH}_2\text{-O} \end{array}$$

IT 663198-00-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (design, synthesis and structure-Activity relationships of dual inhibitors of acetylcholinesterase and serotonin transporter as potential agents for Alzheimer's disease)

RN 663198-00-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(ethylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

GI

AB We have designed and synthesized a dual inhibitor of acetylcholinesterase (AChE) and serotonin transporter (SERT) as a novel class of treatment drugs for Alzheimer's disease on the basis of a hypothetical model of the AChE active site. Dual inhibitions of AChE and SERT would bring about greater therapeutic effects than AChE inhibition alone and avoid adverse peripheral effects caused by excessive AChE inhibition. Compound (I) exhibited potent inhibitory activities against AChE (IC50=101 nM) and SERT (IC50=42 nM). Furthermore, I showed inhibitory activities of both AChE and SERT in mice brain following oral administration.

REFERENCE COUNT: 24

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:667576 CAPLUS

DOCUMENT NUMBER: 137:337771

TITLE: Design and Synthesis of Dual Inhibitors of

Acetylcholinesterase and Serotonin Transporter Targeting Potential Agents for Alzheimer's Disease

AUTHOR(S): Kogen, Hiroshi; Toda, Narihiro; Tago, Keiko; Marumoto,

Shinji; Takami, Kazuko; Ori, Mayuko; Yamada, Naho; Koyama, Kazuo; Naruto, Shunji; Abe, Kazumi; Yamazaki, Reina; Hara, Takao; Aoyagi, Atsushi; Abe, Yasuyuki;

Kaneko, Tsugio

CORPORATE SOURCE: Research Information Department, Exploratory Chemistry

Research Laboratories, Neuroscience and Immunology Research Laboratories, Sankyo Co., Ltd., Shinagawa-ku,

Tokyo, 140-8710, Japan

SOURCE: Organic Letters (2002), 4(20), 3359-3362

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:337771

IT 474296-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

Page 27

(Reactant or reagent)

(determination of absolute stereochem. of (dimethylcarbamoyl) (nitrophenoxyethyl)ben

zylamine, prepared as dual acetylcholinesterase/serotonin transporter inhibitor for Alzheimer's disease)

RN 474296-05-4 CAPLUS

CN Methanesulfonic acid, trifluoro-, 5-[[(dimethylamino)carbonyl]oxy]-2-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# IT 444644-93-3P 474295-89-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of chiral (dimethylcarbamoyl) (nitrophenoxyethyl) benzylamine and (dimethylcarbamoyl) (nitrophenoxyethyl) dihydrobenzazepine as dual acetylcholinesterase/serotonin transporter inhibitors for Alzheimer's disease)

RN 444644-93-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 474295-89-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-(methylamino)-3-(4nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 444646-40-6P 444667-96-3P 474295-88-0P 474295-96-0P 474295-97-1P 474295-98-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of chiral (dimethylcarbamoyl) (nitrophenoxyethyl) benzylamine and (dimethylcarbamoyl) (nitrophenoxyethyl) dihydrobenzazepine as dual acetylcholinesterase/serotonin transporter inhibitors for Alzheimer's disease)

RN 444646-40-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 444667-96-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474295-88-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474295-96-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]-3-(methoxymethoxy)phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474295-97-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]-3-hydroxyphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474295-98-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]-3-ethenylphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$H_2C$$
 $H_2C$ 
 $H_1$ 
 $OBu-t$ 
 $NO_2$ 
 $Me_2N$ 
 $O$ 

GΙ

AB Highly efficient acetylcholinesterase (AChE) and serotonin transporter (SERT) dual inhibitors, I and II, were designed on the basis of the hypothetical model of AChE active site and synthesized. Both compds. showed potent inhibitory activities against AChE and SERT.

Ι

REFERENCE COUNT:

24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:575038 CAPLUS

DOCUMENT NUMBER:

137:140527

TITLE:

Preparation of alkylcarbamic acid esters as

acetylcholinesterase inhibitor and serotonin reuptake

inhibitor

Patent

INVENTOR(S):

Koyama, Kazuo; Marumoto, Shinji; Toda, Narihiro;

Kogen, Hiroshi; Suzuki, Keiko

PATENT ASSIGNEE(S):

Sankyo Company, Limited, Japan

SOURCE:

PCT Int. Appl., 300 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.			KIND DATE				APPL	ICAT:	ION 1		DATE							
WO	20020	0590	 74		A1	-	 2002	0801	1	WO 2	002-	JP40	0		2	0020	122	
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	RW:	AT,		CH,		•		ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	
CA	24358	•	55,	110	AA			0801			002-:					0020		
EP	13628	844			A1		2003	1119		EP 2	002-	7163	23		2	0020	122	
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		ΙE,	FI,	CY,	TR													
JP	2003	1762	56		A2		2003	0624		JP 2	002-	1513	6		2	0020	124	
US	20040	0679	81		A1		2004	0408		US 2	003-	6291	0.8		2	0030	728	
PRIORITY	APP	LN.	INFO	. :						JP 2	001-	1838	6		A 2	0010	126	
										JP 2	001-	3051	82	1	A 2	0011	001	
										WO 2	002-	JP40	0	1	W 2	0020	122	

OTHER SOURCE(S):

MARPAT 137:140527

IT 444644-93-3P 444645-18-5P 444645-78-7P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of alkylcarbamic acid esters as acetylcholinesterase inhibitor)

RN 444644-93-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-

nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 444645-18-5 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(2-chloro-4-nitrophenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \parallel & \\ \text{Me}_2\text{N-C-O} & \\ \hline & \text{NHMe} \\ \hline & \text{CH-CH}_2\text{-CH}_2\text{-O} \\ \hline & \text{C1} \end{array}$$

● HCl

RN 444645-78-7 CAPLUS

CN Carbamic acid, dimethyl-, 2-methyl-4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

IT 444644-44-4P 444644-84-2P 444644-91-1P 444644-96-6P 444645-06-1P 444645-31-2P 444645-79-8P 444667-97-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of alkylcarbamic acid esters as acetylcholinesterase inhibitor)

RN 444644-44-4 CAPLUS CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-

nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NHMe} \\ \text{NHMe} \\ \text{CH-CH}_2\text{-CH}_2\text{-O} \end{array}$$

HCl

RN 444644-84-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(3-fluoro-4-nitrophenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-91-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(2-fluoro-4-nitrophenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \parallel & \\ \text{Me}_2\text{N-C-O} & \\ \hline & \text{NHMe} \\ \hline & \text{CH-CH}_2\text{-CH}_2\text{-O} \\ \hline & \\ & \text{F} \end{array}$$

● HCl

RN 444644-96-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-06-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(3-methyl-4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \text{Me} \\ \text{Me}_2\text{N-C-O} & \text{NHMe} \\ \hline & \text{CH-CH}_2\text{-CH}_2\text{-O} \end{array}$$

HCl

RN 444645-31-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(ethylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-79-8 CAPLUS

CN Carbamic acid, dimethyl-, 2-methyl-4-[(1R)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 444667-97-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 444667-96-3 CMF C19 H23 N3 O5

Absolute stereochemistry.

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

IT 444646-40-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of alkylcarbamic acid esters as acetylcholinesterase inhibitor)

RN 444646-40-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

GI

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB Title compds. [I; R1 = C1-6 alkyl; R2, R3 independently = H, alkyl; Ra = C1-6 alkyl, H; Q = aryl; A = C1-6 alkylene; E = single bond, oxygen, sulfur; X1, X2 independently = oxygen, sulfur], stereoisomers, a pharmacol. acceptable salt, or ester are prepared and are in vitro tested

for acetylcholinesterase inhibition effects. The title compound II·HCl was prepared from dimethylcarbamic acid chloride, 1-(3-hydroxyphenyl)ethanone, 4-(trifluoromethyl)benzaldehyde, and methylamine via condensation reaction. The title compound III·HCl showed acetylcholinesterase inhibition at IC50(nM) = 19 and serotonin reuptake inhibition at IC50(nM) = 6.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file req		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	33.24	194.78
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.38	-4.38

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STRUCTURE FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5 DICTIONARY FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5

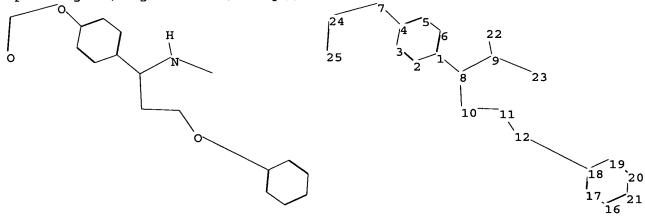
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\106291084.str



chain nodes : 7 8 9 10 11 12 22 23 24 25 ring nodes : 1 2 3 4 5 6 16 17 18 19 20 chain bonds : 1-8 4-7 7-24 8-9 8-10 9-22 9-23 10-11 11-12 12-18 24-25 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 exact/norm bonds : 4-7 7-24 8-9 9-23 11-12 12-18 24-25 exact bonds : 1-8 8-10 9-22 10-11 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 isolated ring systems : containing 1 : G1:0,S G2:0,S,N Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS L5 STRUCTURE UPLOADED => s 15SAMPLE SEARCH INITIATED 17:44:50 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 466 TO ITERATE 9 ANSWERS 466 ITERATIONS 100.0% PROCESSED SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* \*\*COMPLETE\*\* BATCH 8025 TO 10615 PROJECTED ITERATIONS: 9 TO PROJECTED ANSWERS: 360 9 SEA SSS SAM L5 => d scan 9 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN L6 Carbamic acid, dimethyl-, 4-[3-[4-(acetylamino)phenoxy]-1-IN (methylamino)propyl]phenyl ester, monohydrochloride (9CI) C21 H27 N3 O4 . Cl H MF

HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s 15 ful

FULL SEARCH INITIATED 17:45:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 8968 TO ITERATE

100.0% PROCESSED 8968 ITERATIONS 156 ANSWERS

SEARCH TIME: 00.00.01

L7 156 SEA SSS FUL L5

=> file caplus

SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 161.33 356.11 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION 0.00 -4.38 CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 16 Feb 2005 VOL 142 ISS 8 FILE LAST UPDATED: 15 Feb 2005 (20050215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17

L8 6 L7

=> file reg SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION FULL ESTIMATED COST 0.90 357.01 SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) ENTRY SESSION 0.00 -4.38 CA SUBSCRIBER PRICE

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STRUCTURE FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5 DICTIONARY FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5

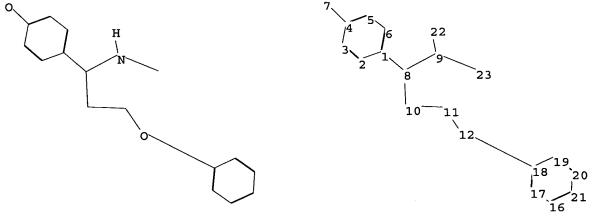
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Uploading C:\Program Files\Stnexp\Queries\106291085.str



chain nodes :

7 8 9 10 11 12 22 23

ring nodes :

1 2 3 4 5 6 16 17 18 19 20 21

chain bonds :

1-8 4-7 8-9 8-10 9-22 9-23 10-11 11-12 12-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 exact/norm bonds :

4-7 8-9 9-23 11-12 12-18

exact bonds :

1-8 8-10 9-22 10-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

isolated ring systems :

containing 1 :

G1:0,S

G2:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS

23:CLASS

STRUCTURE UPLOADED L9

=> s 19

SAMPLE SEARCH INITIATED 17:47:06 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 483 TO ITERATE

100.0% PROCESSED 483 ITERATIONS 9 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

8342 TO 10978 PROJECTED ITERATIONS:

9 TO 360 PROJECTED ANSWERS:

9 SEA SSS SAM L9 L10

=> s 19 ful

FULL SEARCH INITIATED 17:47:15 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 9360 TO ITERATE

100.0% PROCESSED 9360 ITERATIONS 157 ANSWERS

SEARCH TIME: 00.00.01

L11 157 SEA SSS FUL L9

=> file caplus

SINCE FILE TOTAL COST IN U.S. DOLLARS

ENTRY SESSION 161.33 518.34

FULL ESTIMATED COST

SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) TOTAL ENTRY SESSION

-4.38 0.00 CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 16 Feb 2005 VOL 142 ISS 8 FILE LAST UPDATED: 15 Feb 2005 (20050215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 111 L12 6 L11

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=> file reg SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION 519.69 FULL ESTIMATED COST 1.35 SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SESSION ENTRY 0.00 -4.38

FILE 'REGISTRY' ENTERED AT 17:48:52 ON 16 FEB 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

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15 FEB 2005 HIGHEST RN 831913-30-5 STRUCTURE FILE UPDATES: DICTIONARY FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\106291086.str

chain nodes :
7 8 9 10 11 12 16 17

ring nodes :
1 2 3 4 5 6

chain bonds :
1-8 4-7 8-9 8-10 9-16 9-17 10-11 11-12

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :
4-7 8-9 9-17 11-12

exact bonds :
1-8 8-10 9-16 10-11

normalized bonds :

G1:0,S

G2:0,S,N

Match level :

containing 1 :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 16:CLASS 17:CLASS

21 ANSWERS

L13 STRUCTURE UPLOADED

1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems :

=> s 113

SAMPLE SEARCH INITIATED 17:49:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6545 TO ITERATE

15.3% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 126050 TO 135750
PROJECTED ANSWERS: 2045 TO 3451

L14 21 SEA SSS SAM L13

=> s 113 ful

FULL SEARCH INITIATED 17:49:15 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 130713 TO ITERATE

100.0% PROCESSED 130713 ITERATIONS SEARCH TIME: 00.00.01

2149 ANSWERS

L15 2149 SEA SSS FUL L13

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 161.33 681.02

SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) TOTAL ENTRY SESSION 0.00 -4.38 CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 16 Feb 2005 VOL 142 ISS 8 FILE LAST UPDATED: 15 Feb 2005 (20050215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 115

L16 309 L15

=> log y

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 681.92 FULL ESTIMATED COST 0.90

SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) ENTRY SESSION -4.38 CA SUBSCRIBER PRICE 0.00

STN INTERNATIONAL LOGOFF AT 17:50:27 ON 16 FEB 2005